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Monte Carlo simulation of quantum dots formation during heteroepitaxy

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Abstract. Formation of quantum dots (QD's) during heteroepitaxial growth was investigated by Monte Carlo simulation. Shwoebel barriers for explanation of QD's growth kinetic were suggested. Two different barriers for hops to the upper and lower layers were introduced in our model. Ranges of these barriers for QD's formation were estimated.

Heteroepitaxial growth of highly strained structures offers the possibility to fabricate islands with very narrow size distribution — quantum dots (QD's). The quality, size and uniformity of dots are known to be dependent on deposition conditions [1]. Experimental data indicates Ge island array to be a kinetic-controlled one in contrast to InAs/GaAs system of arrays of 3D coherently strained islands whose formation is governed by thermodynamics [1, 2]. Kinetic theories of ordering emphasize the crucial role of inhomogeneous strain fields in the vicinity of 3D islands. Strain field dependence on island dimensions and deposited dose were demonstrated elsewhere [1, 3]. Strains arising at the interface between substrate and growing island during heteroepitaxial growth as in Ge/Si system are schematically illustrated in Fig. 1.

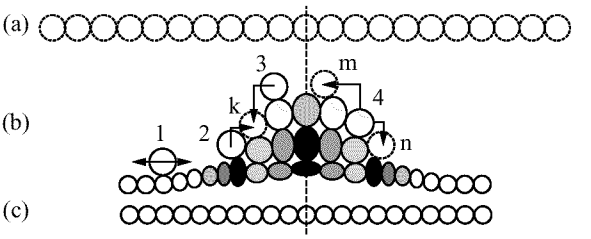

Fig. 1. Schematic drawing illustrating strained heteroepytaxial island (b) of material (a) on the substrate (c) with lattice parameter of lower size. Darker color corresponds to higher stress.

Figure 2 illustrates compression influence on energy for edge atoms in Si_5 cluster. Tersoff potential [4] with parameter [5] was used in our calculation. As could be seen from Fig. 2 energy minimum of atom situated at the origin of the coordinates increases and shifts under pressure. It might be assumed that stress changes binding energy of edge atoms leading to variation of diffusion hops for atoms at tops and walls of 3D islands. We investigate the kinetic of QD's formation during heteroepitaxial growth using standard solid-on-solid (SOS) model [6] as well as 3D model epitaxy on diamond-like crystal (111) surfaces [7]. Monte Carlo simulations of self-assembling process were recently reported [8–11]. However in these works only initial stages of 3D islands growth were considered. We simulated

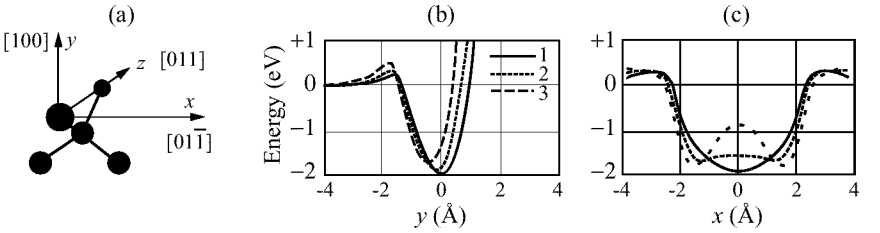

Fig. 2. Schematic draw of Si_5 cluster (a). Si atom under consideration is placed at the origin of the coordinates; Energy dependence on atom position along y direction (b); along x direction (c); (1) — without stress, (2) — linear compression 5%, (3) — linear compression 10%.

3D islands growth during multilayer deposition and took into account peculiarities of edge atoms by introducing additional step edge barrier E_{st} (Schwoebel barrier) in our model. This barrier has to be surmounted by an atom in addition to the surface diffusion barrier if adatom crosses an island edge. So the jump rate to cross an island edge is changed by a factor $P = \exp(-E_{st}/kT)$. Contrary to [10] we introduce two barriers for interlayer hops to the upper layer ($2 \to k$, $4 \to m$) and to the lower layer ($3 \to k$, $4 \to n$) in Fig. 1. Such asymmetry in Schwoebel barrier was found in $Si_{1-x}Ge_x$/Si(001) system [12]. These two barriers correspond to the model parameters P_{up} and P_{down}. P_{up} and P_{down} varied in the following ranges: $0.2 < P_{up} < 5$, $0.1 < P_{down} < 1$ ensuring growth conditions associated with three mechanism of growth: layer-by-layer, 3D island and islands with wet layer growth (Stranski–Krastanov). Values of $P_{up} > 1$ mean that atom hops to the sites in the upper layer is more probable than to the neighbor sites in the same layer.

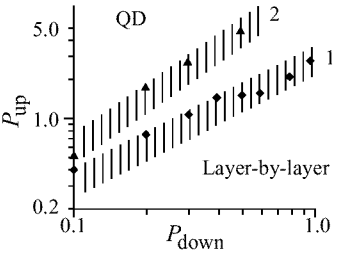

Fig. 3. Phase diagram indicating conditions for three growth mechanisms: shaded area — Stransky–Krastanov (3D islands with wet layer), separating layer-by-layer regime from 3D islands regime was calculated using SOS cubic model (1) and 3D diamond-like model (2).

Crosshatched region in Fig. 3 corresponds to Stranski–Krasstanov growth mechanism while area lower shaded region is consistent with layer-by-layer growth and higher — with QD's formation. Region (1) was obtained using SOS model for cubic crystal and region (2) using 3D model for diamond-like crystal. 3D islands appear only for $P_{down} < 1$, and no 3D are grown for $P_{down} > 1$, even for $P_{up}/P_{down} > 1$. For the shaded region QD's formation takes place after some dose deposition. At the initial stage of growth islands of the second layer appear after coalescence of the first layer islands. Ratio of whole number of up hopping atoms to down hopping ones increases with time. This increase results from the fact that not only P_{up}/P_{down} value determine 3D islands formation but numbers of up, down or lateral target sites for hopping atoms. Rather sharp size distribution of 3D islands observed in Fig. 4(c) (in comparison with Fig. 4(b)) is due to nucleation in the second layer

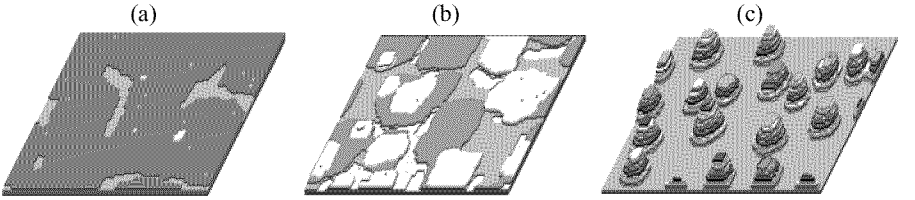

Fig. 4. The simulated surfaces (160 × 160 atomic sites) using SOS model after 1.9 ML deposition for adatom diffusion length $\lambda = 20$ a.s., $b = 0.01$ (parameter $b = \exp(-E_b/kT)$ determines bond energy E_b for given temperature) (a) $P_{up} = 1$, $P_{down} = 1$; (b) $P_{up} = 0.8$, $P_{down} = 0.2$; (c) $P_{up} = 1$, $P_{down} = 0.1$.

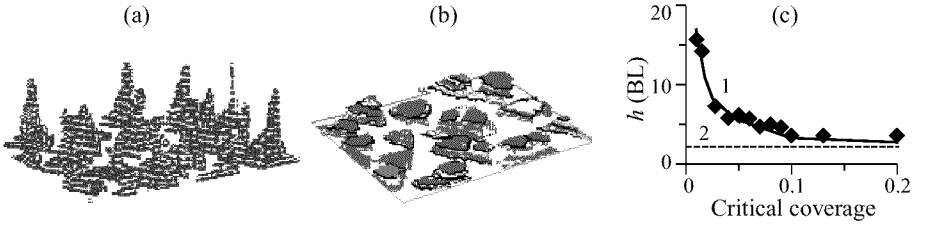

Fig. 5. The simulated surfaces (100 × 100 atomic sites) using 3D model after 2 ML deposition at $T = 725$ K, $P_{up} = 3$, $P_{down} = 0.3$: (a) critical coverage $\Theta_{cr} = 0.01$; (b) $\Theta_{cr} = 0.1$; (c) (1) — average 3D islands height dependence on Θ_{cr}, (2) — thickness of flat film.

before coalescence of islands in the first layer. Islands nucleated earlier are distributed more uniform.

Figure 5 demonstrates simulation results of QD's formation using 3D model for diamond-like crystal. Dependence of Schwoebel barrier on layer number was not taken into account in these calculations. However barrier dependence on average size of island was introduced in 3D model. We suggested barrier to be dependent on deposited dose in the following way: $P(\Theta) = [(P_0 - 1)/\Theta_{cr}] \cdot \Theta + 1$ for $\Theta < \Theta_{cr}$ and $P(\Theta) = P_0$ for $\Theta > \Theta_{cr}$, where $P_0 = \exp(-E_{st}/kT)$, Θ is layer coverage, Θ_{cr} is critical layer coverage. After 2 ML deposition with Schwoebel barriers corresponding to $P_{0up} = 3$ and $P_{0down} = 0.3$ quiet different 3D islands appear for two different Θ_{cr}. If P achieves it's maximum value P_0 after 1% monolayer coverage we get rather high sharp islands (Fig. 5(a)) and if $P = P_0$ after 10% monolayer coverage — islands become flatter (Fig. 5(b)). Dependence of average islands height on critical coverage Θ_{cr} is shown in Fig. 5(c), curve 1. Curve 2 corresponds to film thickness in the case of layer-by-layer growth. Later on we are going to introduce barrier dependence on atomic layer number of growing island.

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